

Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09011**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 5:12:57 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric Result

logP (XH +) -4.95 ±1.76 (n=49)
 logP (neutral X) 2.87 ±0.01 (n=49)
 RMSD 0.236

18C-09011 Points 2 to 18

M13_octanol concentration factor 0.835
 Carbonate 0.0000 mM
 Acidity error 3.14531 mM

18C-09011 Points 19 to 34

M13_octanol concentration factor 0.903
 Carbonate 0.0000 mM
 Acidity error 3.32532 mM

18C-09011 Points 35 to 65

M13_octanol concentration factor 0.690
 Carbonate 0.2248 mM
 Acidity error 3.00531 mM

Warnings and errors

Errors None
 Warnings One or more logP values out of range

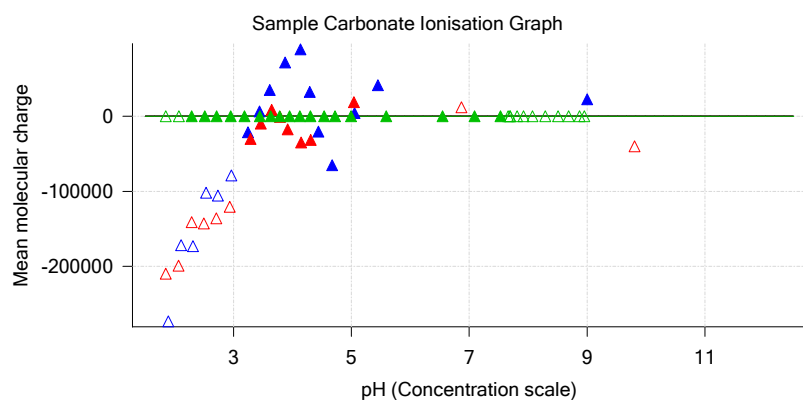
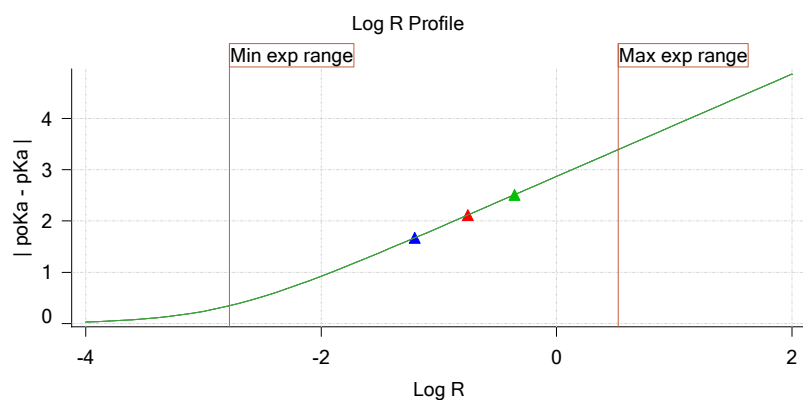
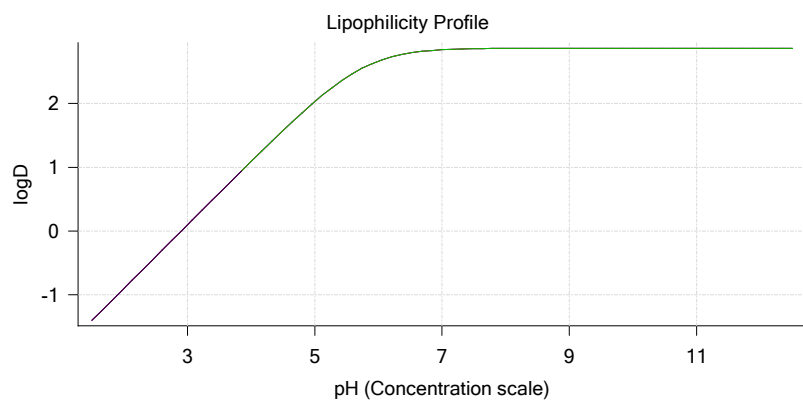
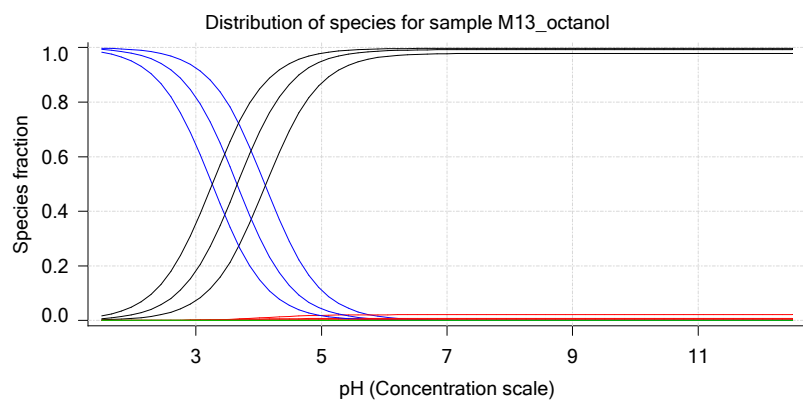
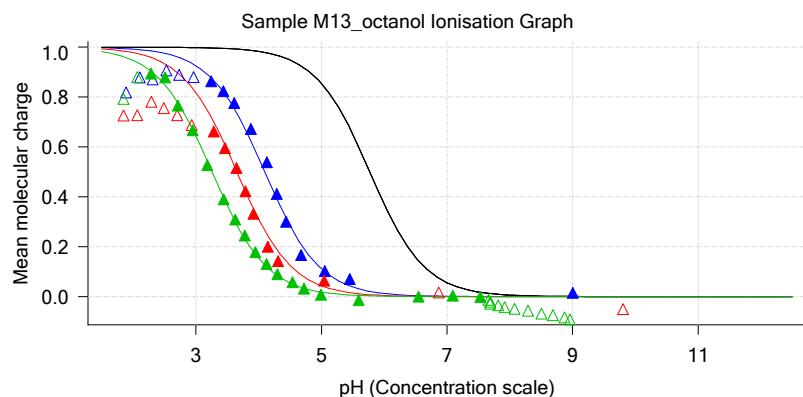
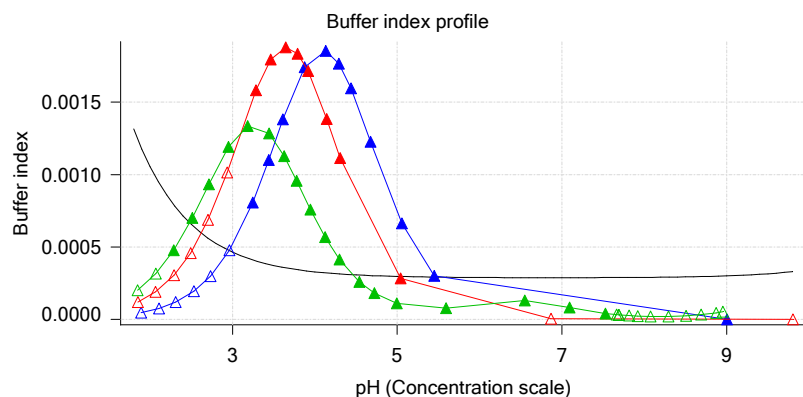
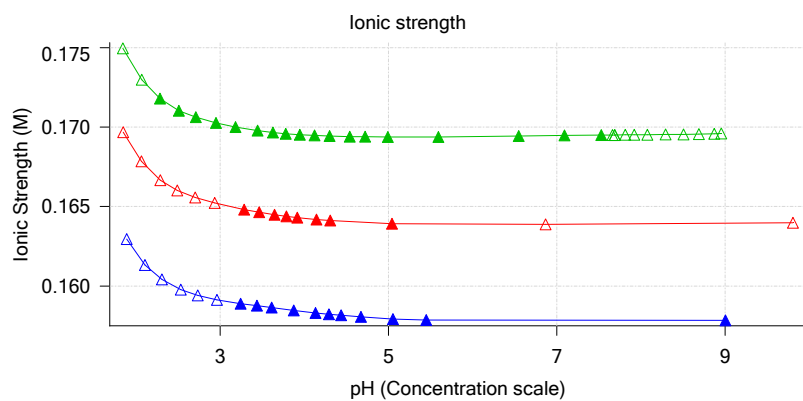
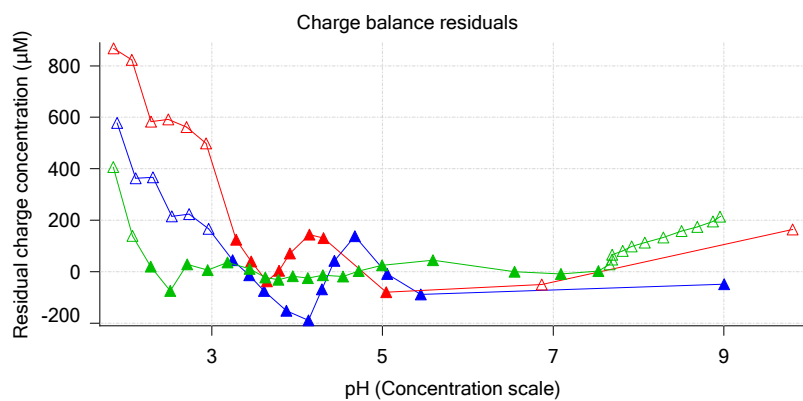
Sample logD and percent species

pH	M13_octanol logD	M13_octanol M13_octanolH	M13_octanol M13_octanol	M13_octanol M13_octanolH*	M13_octanol M13_octanol*	Comment
1.000	-1.90	98.76 %	0.00 %	0.00 %	1.24 %	Stomach pH
1.200	-1.70	98.05 %	0.00 %	0.00 %	1.95 %	
2.000	-0.90	88.86 %	0.02 %	0.00 %	11.13 %	
3.000	0.10	44.37 %	0.08 %	0.00 %	55.56 %	
4.000	1.09	7.39 %	0.13 %	0.00 %	92.49 %	
5.000	2.03	0.79 %	0.13 %	0.00 %	99.07 %	Blood pH
6.000	2.67	0.08 %	0.14 %	0.00 %	99.78 %	
6.500	2.79	0.03 %	0.14 %	0.00 %	99.84 %	
7.000	2.84	0.01 %	0.14 %	0.00 %	99.86 %	
7.400	2.86	0.00 %	0.14 %	0.00 %	99.86 %	
8.000	2.87	0.00 %	0.14 %	0.00 %	99.86 %	
9.000	2.87	0.00 %	0.14 %	0.00 %	99.86 %	
10.000	2.87	0.00 %	0.14 %	0.00 %	99.86 %	
11.000	2.87	0.00 %	0.14 %	0.00 %	99.86 %	
12.000	2.87	0.00 %	0.14 %	0.00 %	99.86 %	

Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09011**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

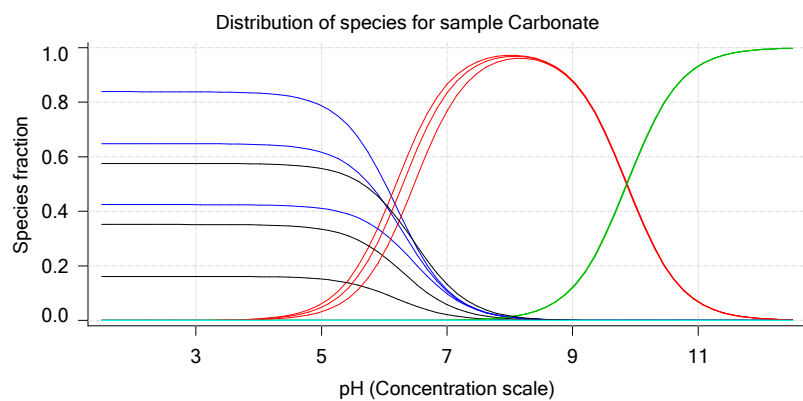
Experiment start time: **3/9/2018 5:12:57 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Graphs



Sample name:	M13_octanol	Experiment start time:	3/9/2018 5:12:57 PM
Assay name:	pH-metric high logP	Analyst:	Pion
Assay ID:	18C-09011	Instrument ID:	T312060
Filename:	C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r		

Graphs (continued)



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09011**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 5:12:57 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 1 of 3 18C-09011 Points 2 to 18

Overall results

RMSD 0.383
 Average ionic strength 0.158 M
 Average temperature 24.9°C
 Partition ratio 0.0624 : 1
 Analyte concentration range 3623.6 µM to 3730.0 µM
 Total points considered 11 of 17

Warnings and errors

Errors None
 Warnings One or more logP values out of range
 Excessive acidity error present

Four-Plus parameters

Alpha 0.102 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r
 S 0.9967 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r
 jH 1.2 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r
 jOH 0.0 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r

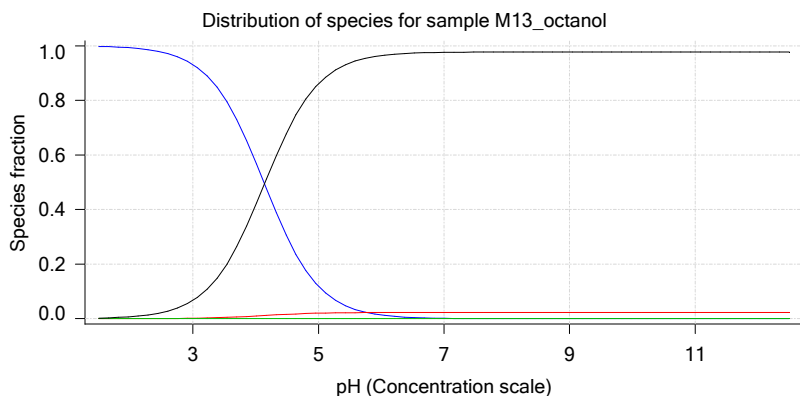
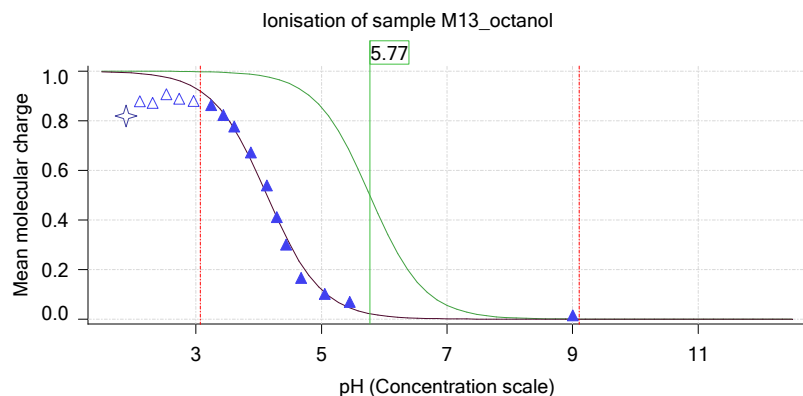
Titrants

0.50 M HCl 0.999843 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r
 0.50 M KOH 0.999845 3/9/2018 5:12:57 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M13_octanol concentration factor 0.835
 Base pKa 1 5.77
 logP (XH +) -4.56
 logP (neutral X) 2.83

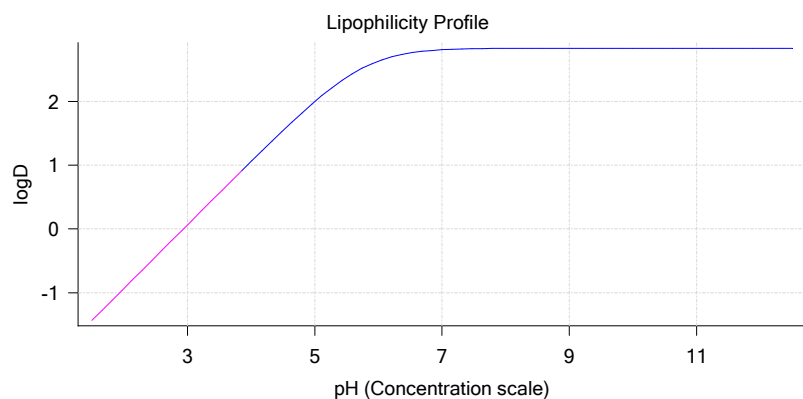
Sample graphs



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09011**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 5:12:57 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Sample graphs (continued)



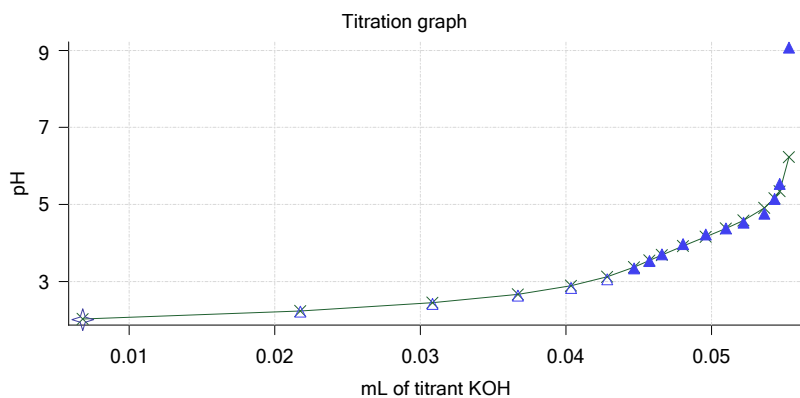
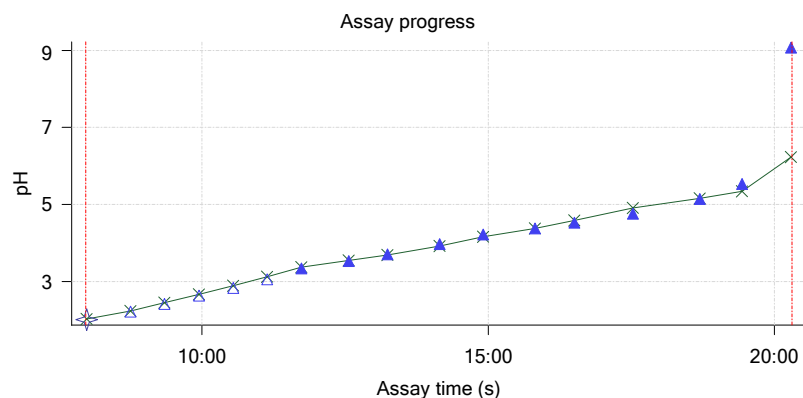
Sample logD and percent species

pH	M13_octanol logD	M13_octanol M13_octanolH	M13_octanol M13_octanolH	M13_octanol M13_octanolH*	M13_octanol M13_octanol*	Comment
1.000	-1.94	99.93 %	0.00 %	0.00 %	0.07 %	Stomach pH
1.200	-1.74	99.88 %	0.00 %	0.00 %	0.11 %	
2.000	-0.94	99.27 %	0.02 %	0.00 %	0.72 %	
3.000	0.06	93.11 %	0.16 %	0.00 %	6.73 %	
4.000	1.06	57.49 %	0.98 %	0.00 %	41.53 %	
5.000	2.00	11.91 %	2.02 %	0.00 %	86.06 %	Blood pH
6.000	2.63	1.33 %	2.27 %	0.00 %	96.40 %	
6.500	2.76	0.43 %	2.29 %	0.00 %	97.29 %	
7.000	2.81	0.14 %	2.29 %	0.00 %	97.57 %	
7.400	2.82	0.05 %	2.30 %	0.00 %	97.65 %	
8.000	2.83	0.01 %	2.30 %	0.00 %	97.69 %	
9.000	2.83	0.00 %	2.30 %	0.00 %	97.70 %	
10.000	2.83	0.00 %	2.30 %	0.00 %	97.70 %	
11.000	2.83	0.00 %	2.30 %	0.00 %	97.70 %	
12.000	2.83	0.00 %	2.30 %	0.00 %	97.70 %	

Carbonate and acidity

Carbonate 0.000 mM
 Acidity error 3.145 mM

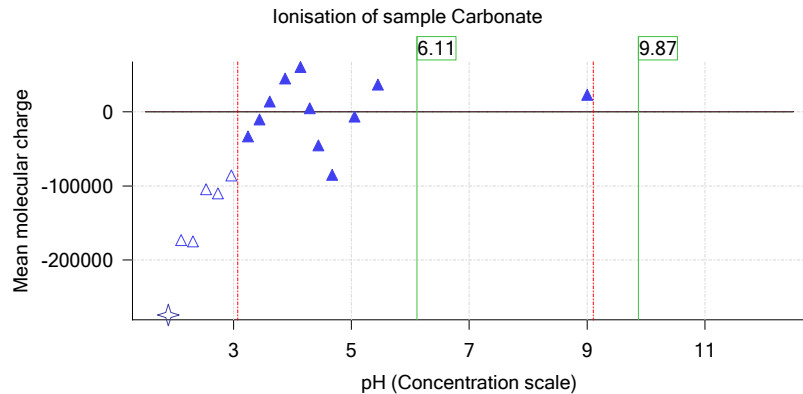
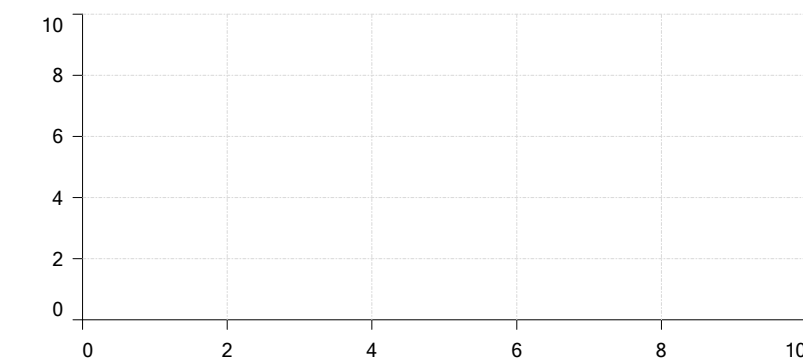
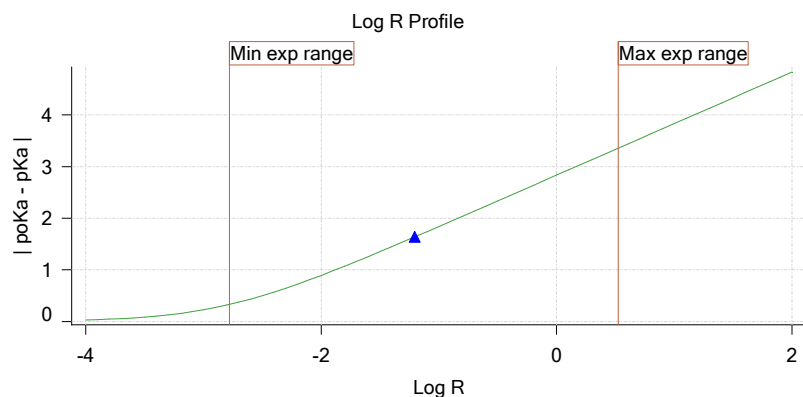
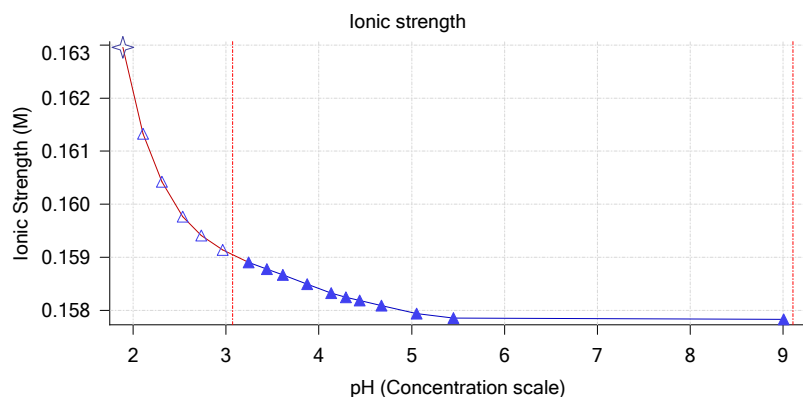
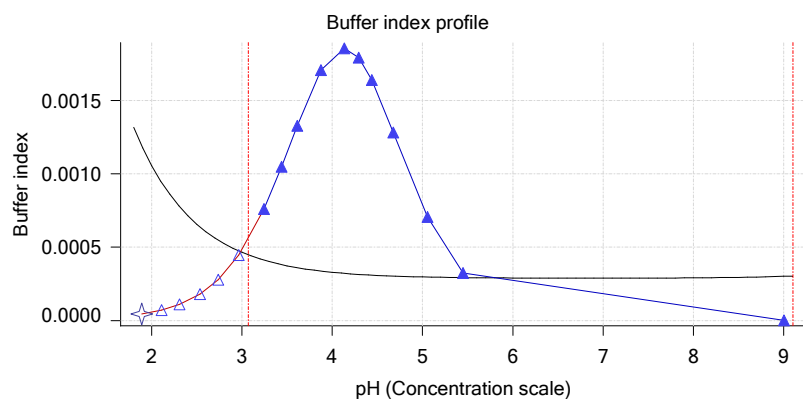
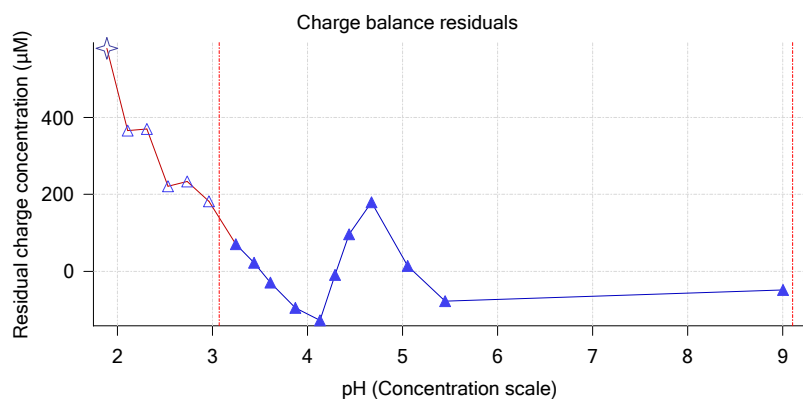
Other graphs



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09011**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 5:12:57 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09011**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 5:12:57 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 2 of 3 18C-09011 Points 19 to 34

Overall results

RMSD 0.118
 Average ionic strength 0.164 M
 Average temperature 24.9°C
 Partition ratio 0.1757 : 1
 Analyte concentration range 3064.9 µM to 3153.0 µM
 Total points considered 8 of 16

Warnings and errors

Errors None
 Warnings One or more logP values out of range
 Excessive acidity error present

Four-Plus parameters

Alpha 0.102 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r
 S 0.9967 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r
 jH 1.2 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r
 jOH 0.0 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r

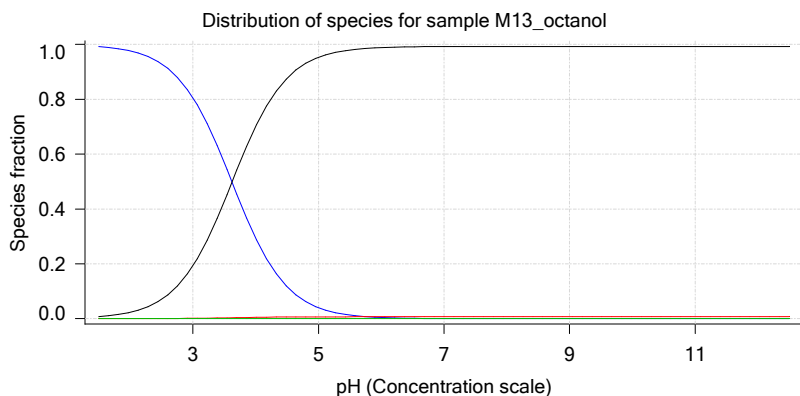
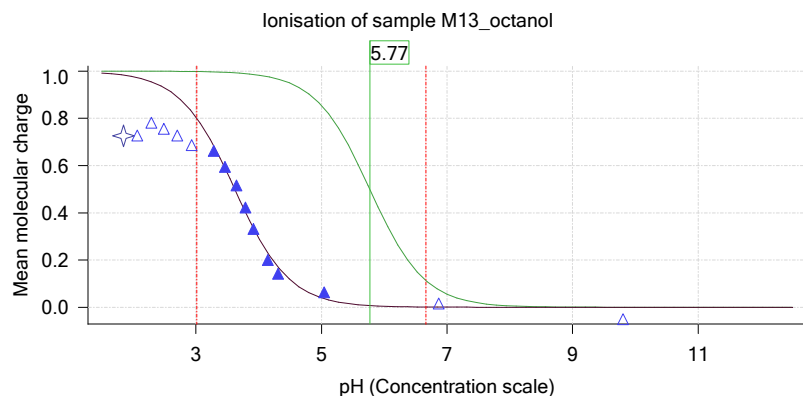
Titrants

0.50 M HCl 0.999843 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r
 0.50 M KOH 0.999845 3/9/2018 5:12:57 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M13_octanol concentration factor 0.903
 Base pKa 1 5.77
 logP (XH +) -4.56
 logP (neutral X) 2.90

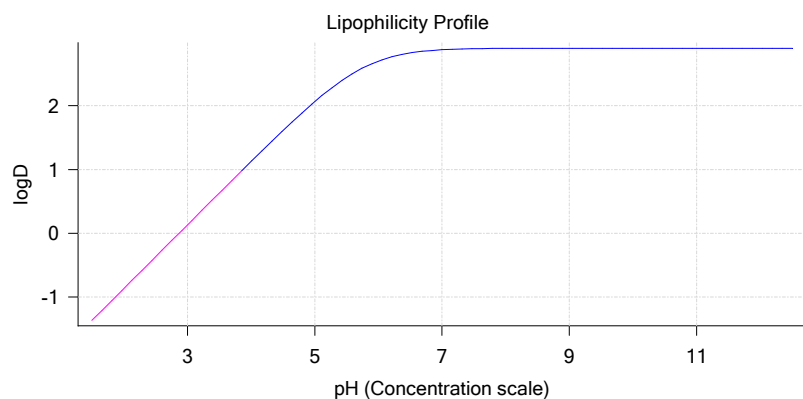
Sample graphs



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09011**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 5:12:57 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Sample graphs (continued)



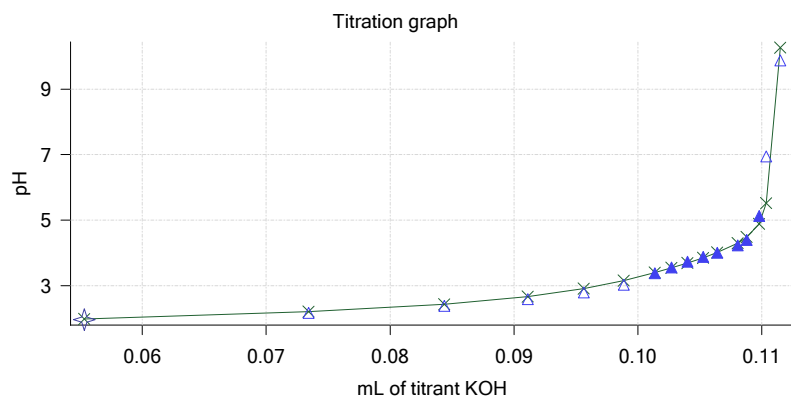
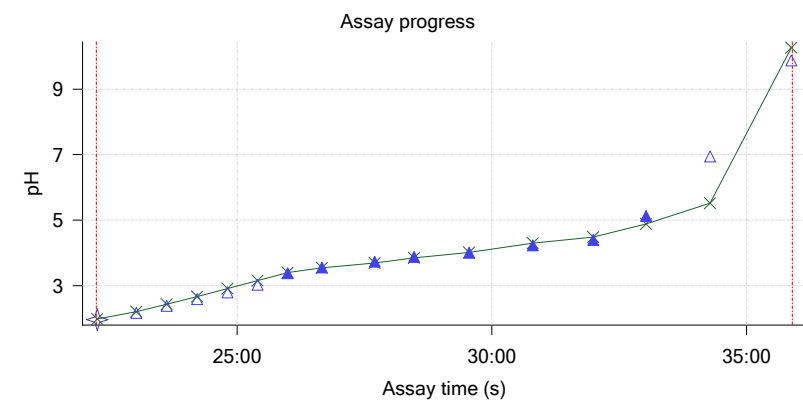
Sample logD and percent species

pH	M13_octanol logD	M13_octanol M13_octanolH	M13_octanol M13_octanolH	M13_octanol M13_octanolH*	M13_octanol M13_octanol*	Comment
1.000	-1.87	99.76 %	0.00 %	0.00 %	0.24 %	Stomach pH
1.200	-1.67	99.62 %	0.00 %	0.00 %	0.38 %	
2.000	-0.87	97.66 %	0.02 %	0.00 %	2.33 %	
3.000	0.13	80.65 %	0.14 %	0.00 %	19.21 %	
4.000	1.13	29.42 %	0.50 %	0.00 %	70.08 %	
5.000	2.06	4.00 %	0.68 %	0.00 %	95.32 %	Blood pH
6.000	2.70	0.42 %	0.70 %	0.00 %	98.88 %	
6.500	2.83	0.13 %	0.71 %	0.00 %	99.16 %	
7.000	2.88	0.04 %	0.71 %	0.00 %	99.25 %	
7.400	2.89	0.02 %	0.71 %	0.00 %	99.28 %	
8.000	2.90	0.00 %	0.71 %	0.00 %	99.29 %	
9.000	2.90	0.00 %	0.71 %	0.00 %	99.29 %	
10.000	2.90	0.00 %	0.71 %	0.00 %	99.29 %	
11.000	2.90	0.00 %	0.71 %	0.00 %	99.29 %	
12.000	2.90	0.00 %	0.71 %	0.00 %	99.29 %	

Carbonate and acidity

Carbonate 0.000 mM
 Acidity error 3.325 mM

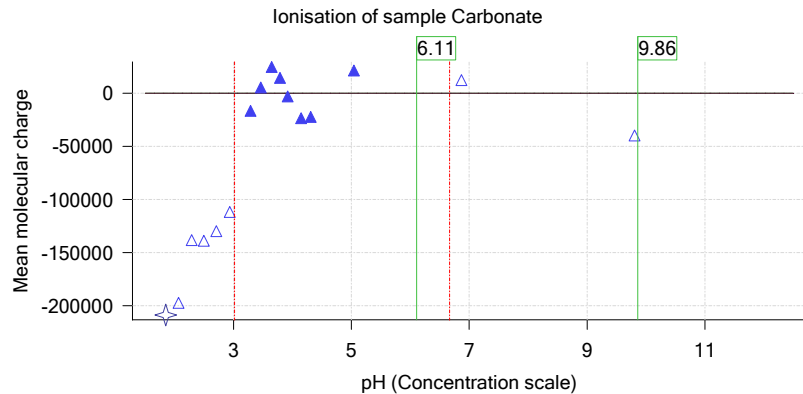
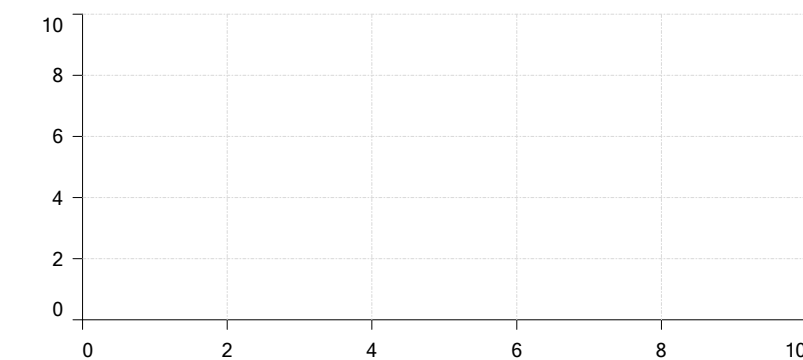
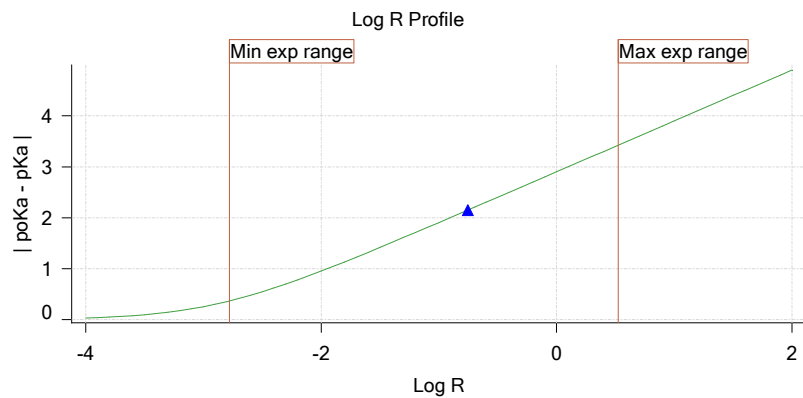
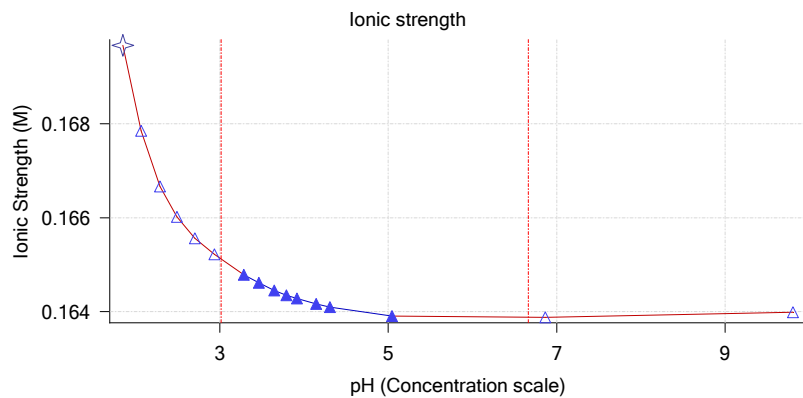
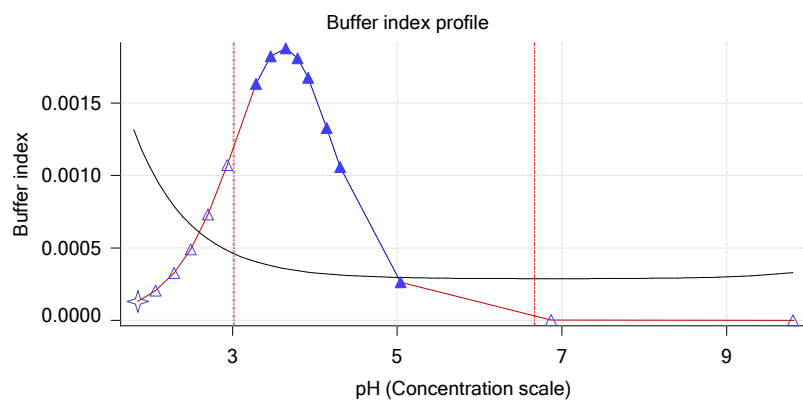
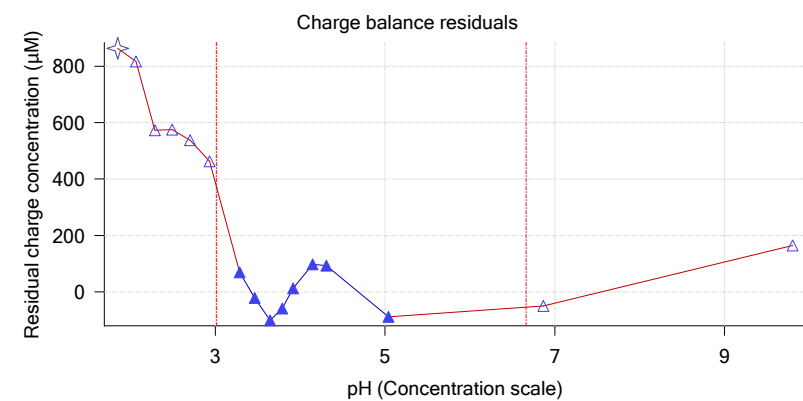
Other graphs



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 Assay ID: **18C-09011**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 5:12:57 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09011**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 5:12:57 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 3 of 3 18C-09011 Points 35 to 65

Overall results

RMSD 0.137
 Average ionic strength 0.170 M
 Average temperature 25.0°C
 Partition ratio 0.4387 : 1
 Analyte concentration range 2344.1 µM to 2398.3 µM
 Total points considered 18 of 31

Warnings and errors

Errors None
 Warnings Sample concentration factor out of range
 One or more logP values out of range
 Excessive acidity error present

Four-Plus parameters

Alpha 0.102 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r
 S 0.9967 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r
 jH 1.2 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r
 jOH 0.0 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r

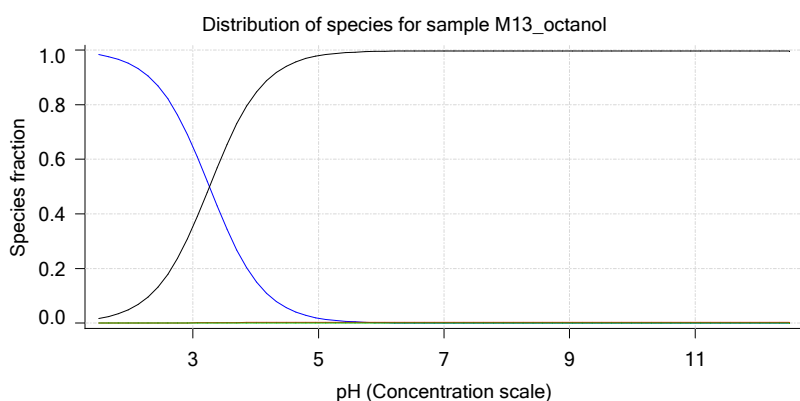
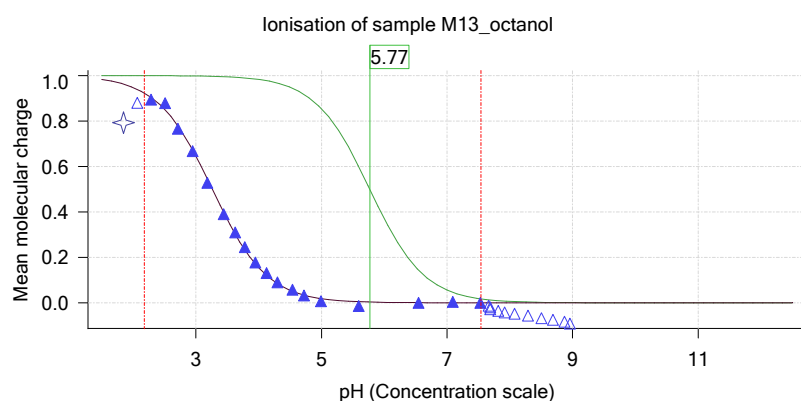
Titrants

0.50 M HCl 0.999843 3/9/2018 5:12:57 PM C:\Sirius_T3\HCl18C09.t3r
 0.50 M KOH 0.999845 3/9/2018 5:12:57 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M13_octanol concentration factor 0.690
 Base pKa 1 5.77
 logP (XH +) -4.56
 logP (neutral X) 2.86

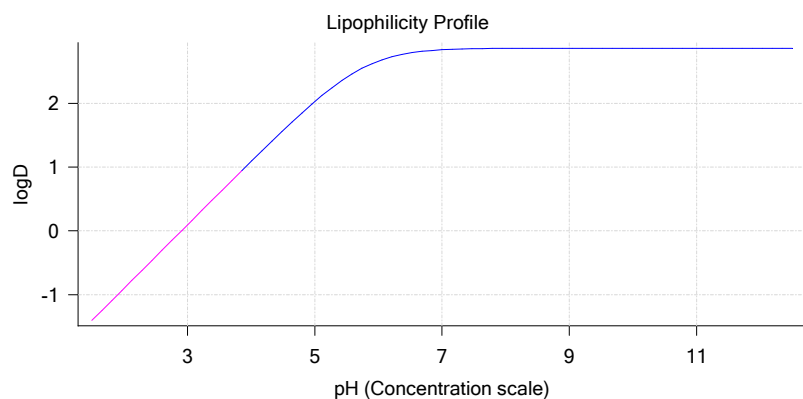
Sample graphs



Sample name: **M13_octanol**
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 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 5:12:57 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Sample graphs (continued)



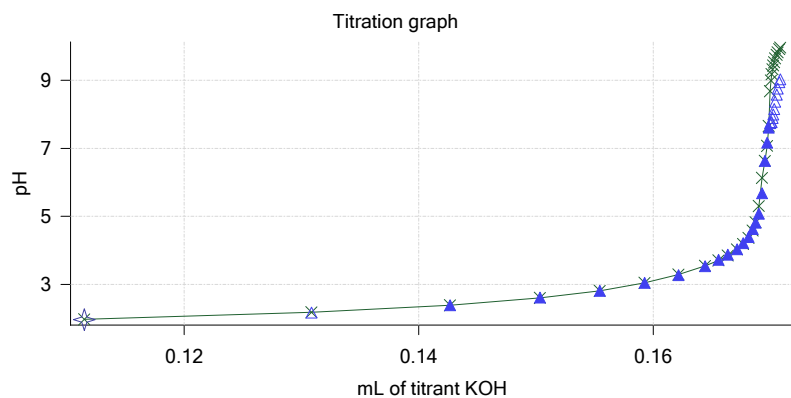
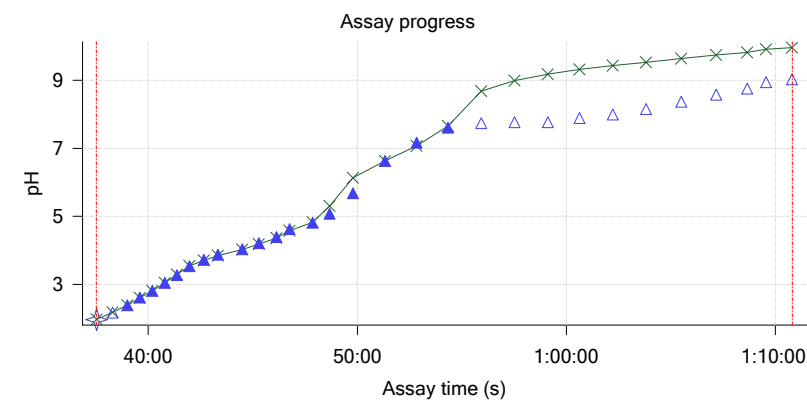
Sample logD and percent species

pH	M13_octanol logD	M13_octanol M13_octanolH	M13_octanol M13_octanolH	M13_octanol M13_octanolH*	M13_octanol M13_octanol*	Comment
1.000	-1.90	99.46 %	0.00 %	0.00 %	0.54 %	Stomach pH
1.200	-1.71	99.14 %	0.00 %	0.00 %	0.86 %	
2.000	-0.91	94.82 %	0.02 %	0.00 %	5.17 %	
3.000	0.09	64.66 %	0.11 %	0.00 %	35.23 %	
4.000	1.09	15.47 %	0.26 %	0.00 %	84.27 %	
5.000	2.03	1.80 %	0.31 %	0.00 %	97.90 %	Blood pH
6.000	2.66	0.18 %	0.31 %	0.00 %	99.51 %	
6.500	2.79	0.06 %	0.31 %	0.00 %	99.63 %	
7.000	2.84	0.02 %	0.31 %	0.00 %	99.67 %	
7.400	2.85	0.01 %	0.31 %	0.00 %	99.68 %	
8.000	2.86	0.00 %	0.31 %	0.00 %	99.69 %	
9.000	2.86	0.00 %	0.31 %	0.00 %	99.69 %	
10.000	2.86	0.00 %	0.31 %	0.00 %	99.69 %	
11.000	2.86	0.00 %	0.31 %	0.00 %	99.69 %	
12.000	2.86	0.00 %	0.31 %	0.00 %	99.69 %	

Carbonate and acidity

Carbonate 0.225 mM
 Acidity error 3.005 mM

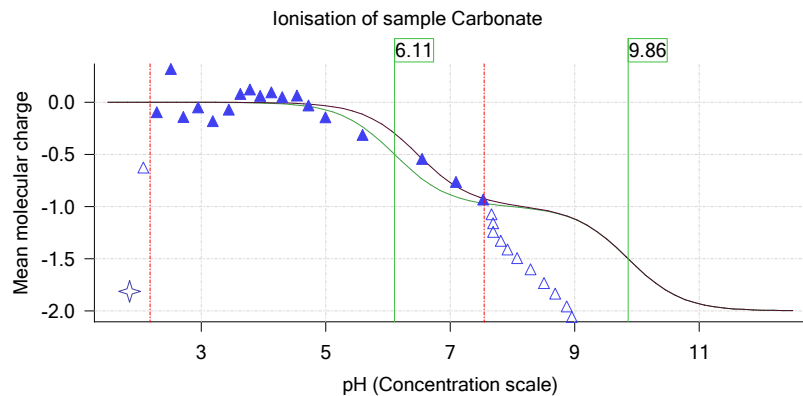
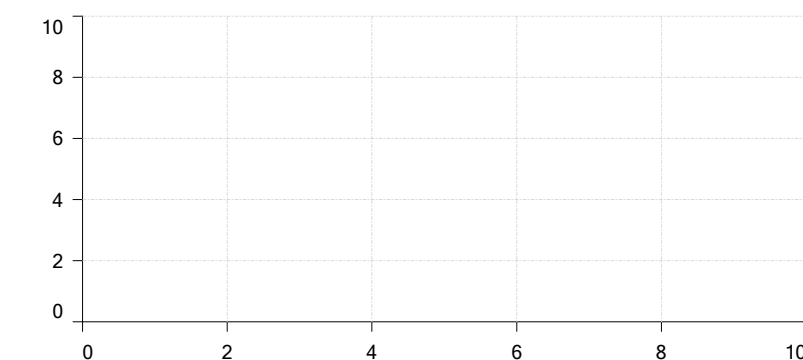
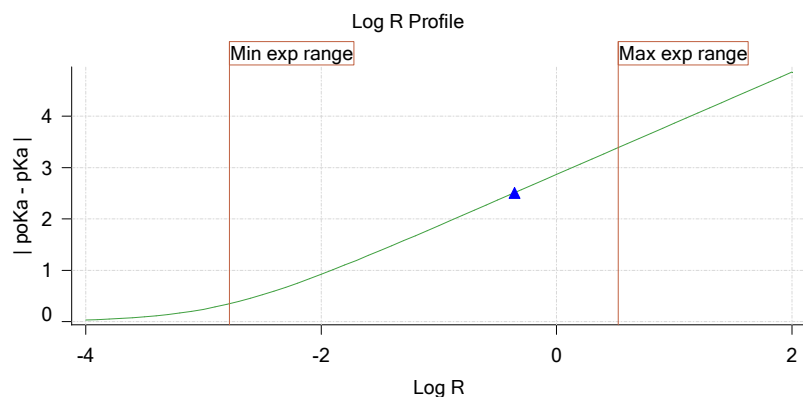
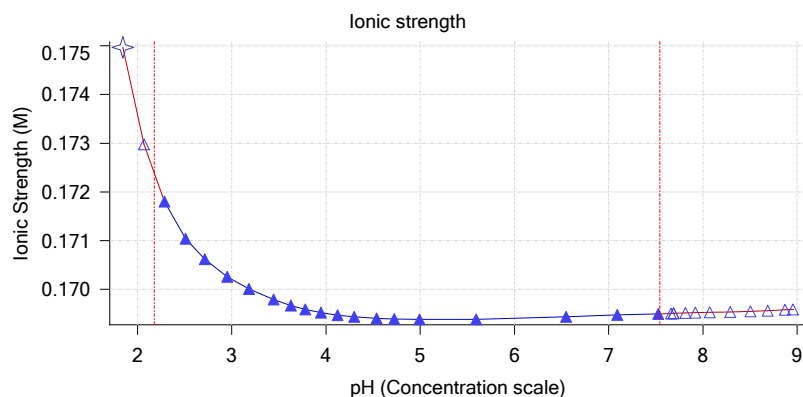
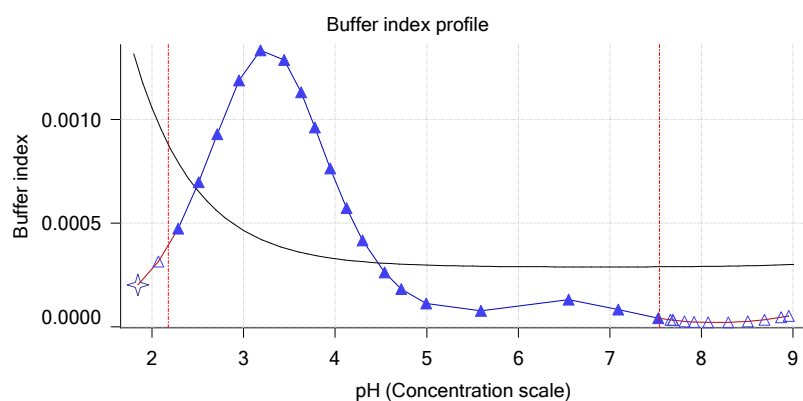
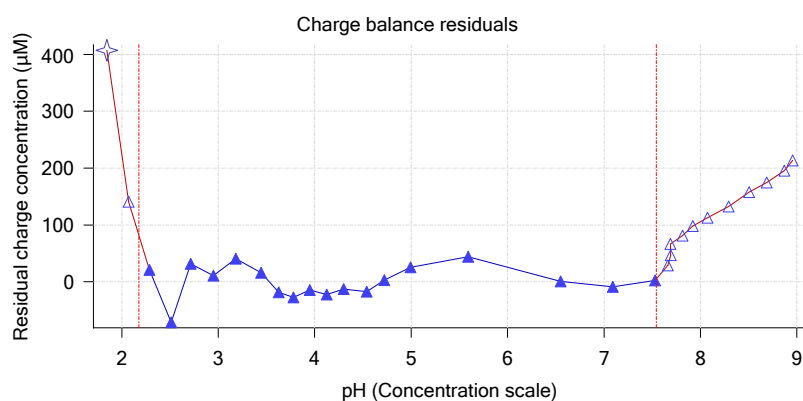
Other graphs



Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09011**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 5:12:57 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)





Assay model

Sample name: **M13_octanol** Experiment start time: **3/9/2018 5:12:57 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-09011** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M13_octanol	2/27/2018 5:57:49 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001820 g	3/9/2018 2:22:18 PM	User entered value
Formula weight	295.34 g/mol	2/27/2018 5:57:49 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	295.34	2/27/2018 5:57:49 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 5:57:49 PM	User entered value
Sample is a	Base	2/27/2018 5:57:49 PM	User entered value
pKa 1	5.77	2/27/2018 5:57:49 PM	User entered value
logp (XH +)	-4.56	3/2/2018 4:30:48 PM	User entered value
logP (neutral X)	2.99	3/2/2018 4:30:43 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/ time
4:58.3	Manual volume addition				0.10000 mL					
4:59.4	Initial pH = 4.15									
7:58.9	Data point 2	1.50000 mL	0.04534 mL	0.00680 mL	0.10000 mL	2.003	-0.00733	0.78688	0.00041	10.0 s
8:45.1	Data point 3	1.50000 mL	0.04534 mL	0.02175 mL	0.10000 mL	2.213	-0.00482	0.44185	0.00036	10.0 s
9:20.7	Data point 4	1.50000 mL	0.04534 mL	0.03083 mL	0.10000 mL	2.410	-0.00055	0.04460	0.00013	10.5 s
9:56.8	Data point 5	1.50000 mL	0.04534 mL	0.03669 mL	0.10000 mL	2.631	-0.00364	0.36884	0.00030	10.5 s
10:32.8	Data point 6	1.50000 mL	0.04534 mL	0.04033 mL	0.10000 mL	2.831	-0.01005	0.38801	0.00080	10.0 s
11:08.3	Data point 7	1.50000 mL	0.04534 mL	0.04283 mL	0.10000 mL	3.058	-0.01425	0.84558	0.00077	10.5 s
11:44.3	Data point 8	1.50000 mL	0.04534 mL	0.04466 mL	0.10000 mL	3.338	-0.01848	0.91945	0.00095	19.0 s
12:33.9	Data point 9	1.50000 mL	0.04534 mL	0.04572 mL	0.10000 mL	3.531	-0.01812	0.81824	0.00099	10.0 s
13:14.4	Data point 10	1.50000 mL	0.04534 mL	0.04659 mL	0.10000 mL	3.703	-0.01908	0.89474	0.00100	19.0 s
14:09.3	Data point 11	1.50000 mL	0.04534 mL	0.04802 mL	0.10000 mL	3.965	-0.01908	0.89676	0.00099	20.0 s
14:54.7	Data point 12	1.50000 mL	0.04534 mL	0.04960 mL	0.10000 mL	4.221	-0.01943	0.92861	0.00100	19.0 s
15:49.3	Data point 13	1.50000 mL	0.04534 mL	0.05099 mL	0.10000 mL	4.380	-0.01820	0.88224	0.00096	16.0 s
16:30.5	Data point 14	1.50000 mL	0.04534 mL	0.05219 mL	0.10000 mL	4.526	-0.01937	0.97139	0.00097	25.5 s
17:31.9	Data point 15	1.50000 mL	0.04534 mL	0.05362 mL	0.10000 mL	4.762	-0.01918	0.96005	0.00097	34.5 s
18:42.1	Data point 16	1.50000 mL	0.04534 mL	0.05433 mL	0.10000 mL	5.141	-0.01371	0.48473	0.00097	19.0 s
19:26.3	Data point 17	1.50000 mL	0.04534 mL	0.05468 mL	0.10000 mL	5.535	-0.00613	0.11557	0.00089	21.0 s
20:17.7	Data point 18	1.50000 mL	0.04534 mL	0.05532 mL	0.10000 mL	9.077	-0.02136	0.97236	0.00107	Time out at
22:15.2	Data point 19	1.50000 mL	0.09918 mL	0.05532 mL	0.30000 mL	1.963	-0.01099	0.97572	0.00055	10.0 s
23:01.4	Data point 20	1.50000 mL	0.09918 mL	0.07342 mL	0.30000 mL	2.171	-0.01453	0.61507	0.00092	10.0 s



Assay Events

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09011**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 5:12:57 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
23:37.0	Data point 21	1.50000 mL	0.09918 mL	0.08438 mL	0.30000 mL	2.390	0.00209	0.42447	0.00016	10.5 s
24:13.0	Data point 22	1.50000 mL	0.09918 mL	0.09111 mL	0.30000 mL	2.590	-0.00255	0.12562	0.00035	10.0 s
24:48.6	Data point 23	1.50000 mL	0.09918 mL	0.09565 mL	0.30000 mL	2.800	0.00274	0.51472	0.00019	10.0 s
25:24.0	Data point 24	1.50000 mL	0.09918 mL	0.09887 mL	0.30000 mL	3.028	-0.00247	0.23539	0.00025	10.0 s
25:59.5	Data point 25	1.50000 mL	0.09918 mL	0.10136 mL	0.30000 mL	3.378	-0.01613	0.84514	0.00087	10.0 s
26:40.1	Data point 26	1.50000 mL	0.09918 mL	0.10271 mL	0.30000 mL	3.555	-0.01471	0.68891	0.00088	26.5 s
27:42.3	Data point 27	1.50000 mL	0.09918 mL	0.10400 mL	0.30000 mL	3.737	-0.00307	0.05380	0.00065	10.5 s
28:28.5	Data point 28	1.50000 mL	0.09918 mL	0.10527 mL	0.30000 mL	3.879	-0.01698	0.74340	0.00098	29.0 s
29:33.3	Data point 29	1.50000 mL	0.09918 mL	0.10642 mL	0.30000 mL	4.007	-0.01912	0.90936	0.00099	34.0 s
30:48.3	Data point 30	1.50000 mL	0.09918 mL	0.10807 mL	0.30000 mL	4.234	-0.01945	0.95903	0.00098	40.5 s
31:59.4	Data point 31	1.50000 mL	0.09918 mL	0.10880 mL	0.30000 mL	4.397	-0.01934	0.97445	0.00097	31.5 s
33:01.6	Data point 32	1.50000 mL	0.09918 mL	0.10981 mL	0.30000 mL	5.129	-0.01995	0.97002	0.00100	45.0 s
34:17.2	Data point 33	1.50000 mL	0.09918 mL	0.11037 mL	0.30000 mL	6.946	-0.12491	0.99710	0.00618	Timed out at 59.5 s
35:52.9	Data point 34	1.50000 mL	0.09918 mL	0.11150 mL	0.30000 mL	9.875	-0.00416	0.04424	0.00098	13.5 s
37:31.9	Data point 35	1.50000 mL	0.15807 mL	0.11150 mL	0.80000 mL	1.959	-0.00284	0.16111	0.00035	10.0 s
38:18.1	Data point 36	1.50000 mL	0.15807 mL	0.13086 mL	0.80000 mL	2.175	-0.00636	0.10985	0.00095	16.0 s
38:59.8	Data point 37	1.50000 mL	0.15807 mL	0.14266 mL	0.80000 mL	2.388	-0.01190	0.63324	0.00074	10.0 s
39:35.4	Data point 38	1.50000 mL	0.15807 mL	0.15033 mL	0.80000 mL	2.610	-0.00893	0.81503	0.00049	10.5 s
40:11.5	Data point 39	1.50000 mL	0.15807 mL	0.15543 mL	0.80000 mL	2.809	-0.01069	0.89777	0.00056	10.0 s
40:47.0	Data point 40	1.50000 mL	0.15807 mL	0.15924 mL	0.80000 mL	3.044	-0.00343	0.27090	0.00033	10.0 s
41:22.5	Data point 41	1.50000 mL	0.15807 mL	0.16214 mL	0.80000 mL	3.276	-0.01814	0.88874	0.00095	10.5 s
41:58.5	Data point 42	1.50000 mL	0.15807 mL	0.16439 mL	0.80000 mL	3.535	-0.01802	0.93392	0.00092	10.0 s
42:39.1	Data point 43	1.50000 mL	0.15807 mL	0.16555 mL	0.80000 mL	3.719	-0.01345	0.67807	0.00081	10.0 s
43:19.7	Data point 44	1.50000 mL	0.15807 mL	0.16634 mL	0.80000 mL	3.870	-0.01661	0.94479	0.00084	29.0 s
44:29.7	Data point 45	1.50000 mL	0.15807 mL	0.16712 mL	0.80000 mL	4.037	-0.00694	0.13256	0.00094	11.5 s
45:17.0	Data point 46	1.50000 mL	0.15807 mL	0.16766 mL	0.80000 mL	4.213	0.00141	0.00562	0.00093	10.5 s
46:08.4	Data point 47	1.50000 mL	0.15807 mL	0.16811 mL	0.80000 mL	4.389	-0.01790	0.90016	0.00093	11.5 s
46:45.3	Data point 48	1.50000 mL	0.15807 mL	0.16846 mL	0.80000 mL	4.627	-0.01929	0.94369	0.00098	35.5 s
47:51.4	Data point 49	1.50000 mL	0.15807 mL	0.16872 mL	0.80000 mL	4.810	-0.01458	0.57061	0.00095	19.0 s
48:40.8	Data point 50	1.50000 mL	0.15807 mL	0.16898 mL	0.80000 mL	5.080	-0.01848	0.89699	0.00096	36.0 s
49:47.4	Data point 51	1.50000 mL	0.15807 mL	0.16926 mL	0.80000 mL	5.677	-0.01986	0.97546	0.00099	56.0 s
51:19.2	Data point 52	1.50000 mL	0.15807 mL	0.16950 mL	0.80000 mL	6.630	-0.10160	0.99674	0.00502	Timed out at 59.5 s
52:49.7	Data point 53	1.50000 mL	0.15807 mL	0.16969 mL	0.80000 mL	7.171	-0.11670	0.99695	0.00577	Timed out at 59.5 s
54:20.2	Data point 54	1.50000 mL	0.15807 mL	0.16983 mL	0.80000 mL	7.606	-0.10666	0.99532	0.00527	Timed out at 59.5 s
55:55.8	Data point 55	1.50000 mL	0.15807 mL	0.16994 mL	0.80000 mL	7.740	-0.06542	0.99344	0.00324	Timed out at 59.5 s
57:31.5	Data point 56	1.50000 mL	0.15807 mL	0.17001 mL	0.80000 mL	7.767	-0.04725	0.99135	0.00234	Timed out at 59.5 s
59:07.1	Data point 57	1.50000 mL	0.15807 mL	0.17008 mL	0.80000 mL	7.767	-0.03770	0.96936	0.00189	Timed out at 59.5 s
1:00:37.5	Data point 58	1.50000 mL	0.15807 mL	0.17016 mL	0.80000 mL	7.892	-0.03830	0.97684	0.00191	Timed out at 59.5 s
1:02:13.0	Data point 59	1.50000 mL	0.15807 mL	0.17023 mL	0.80000 mL	7.996	-0.03517	0.97225	0.00176	Timed out at 59.5 s
1:03:48.7	Data point 60	1.50000 mL	0.15807 mL	0.17030 mL	0.80000 mL	8.151	-0.02938	0.97141	0.00147	Timed out at 59.5 s
1:05:29.4	Data point 61	1.50000 mL	0.15807 mL	0.17039 mL	0.80000 mL	8.367	-0.02206	0.95552	0.00111	Timed out at 59.5 s
1:07:10.1	Data point 62	1.50000 mL	0.15807 mL	0.17051 mL	0.80000 mL	8.580	-0.01905	0.91928	0.00098	48.0 s
1:08:39.0	Data point 63	1.50000 mL	0.15807 mL	0.17060 mL	0.80000 mL	8.761	-0.01127	0.33329	0.00096	18.5 s
1:09:33.2	Data point 64	1.50000 mL	0.15807 mL	0.17072 mL	0.80000 mL	8.944	-0.01844	0.86480	0.00098	43.5 s
1:10:47.3	Data point 65	1.50000 mL	0.15807 mL	0.17081 mL	0.80000 mL	9.028	-0.01594	0.74914	0.00091	17.0 s
1:11:13.3	Assay volumes	1.50000 mL	0.15807 mL	0.17081 mL	0.80000 mL					

Sample name: **M13_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-09011**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 5:12:57 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titration Pre-Dose				
Titration pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.100 mL			
Partition solvent added	Manual in advance			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	60 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.200 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M13_octanol** Experiment start time: **3/9/2018 5:12:57 PM**
 Assay name: **pH-metric high logP** Analyst: **Pion**
 Assay ID: **18C-09011** Instrument ID: **T312060**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.500 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.102	3/9/2018 5:12:57 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus S	0.9967	3/9/2018 5:12:57 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus jH	1.2	3/9/2018 5:12:57 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus jOH	0.0	3/9/2018 5:12:57 PM	C:\Sirius_T3\HCl18C09.t3r
Base concentration factor	1.000	3/9/2018 5:12:57 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	1.000	3/9/2018 5:12:57 PM	C:\Sirius_T3\HCl18C09.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 11:05:59 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 11:27:22 AM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 11:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	02-08-2018	3/6/2018 10:28:59 AM
Port B	Cyclohexane	11-01-17	2/27/2018 11:37:57 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 11:18:04 AM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM

Sample name: **M13_octanol** Experiment start time: **3/9/2018 5:12:57 PM**
 Assay name: **pH-metric high logP** Analyst: **Pion**
 Assay ID: **18C-09011** Instrument ID: **T312060**
 Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titration	Octanol	01-31-2018	2/27/2018 10:59:35 AM
Titration		T3TM1200161	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 3:01:00 PM
E0 calibration	+5.90 mV		3/9/2018 5:13:25 PM
Filling solution	3M KCl	KCL097	3/9/2018 11:05:42 AM
Liquids			
Wash 1	50% IPA:50% Water		3/9/2018 11:04:22 AM
Wash 2	0.5% Triton X-100 in H2O		3/9/2018 11:04:25 AM
Buffer position 1	pH7 Wash		3/9/2018 11:04:27 AM
Buffer position 2	pH 7		3/9/2018 11:04:30 AM
Storage position			3/9/2018 11:05:04 AM
Wash water	5.2e+003 mL	02-27-2018	2/27/2018 10:54:39 AM
Waste	1e+004 mL		11/28/2017 11:36:29 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		074811	11/23/2010 12:22:28 PM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	123:16:41		11/23/2010 12:22:28 PM
Calibrated on	2/27/2018 11:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		



Assay Settings

Sample name: **M13_octanol** Experiment start time: **3/9/2018 5:12:57 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-09011** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09011_M13_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00